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12 June 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-AB-2002-140 Karl Christe (ERC) et al., "Nitrogen Fluoride Chemistry" (abstract)

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ACS Meeting

(20 August 2002, Boston, MA)

(Statement A)

Nitrogen Fluoride Chemistry

Ashwani Vij¹, William Wilson¹, Vandana Vij¹, F. Tham², M. Gerken³, and **Karl Christe⁴**. (1) Air Force Research Laboratory, Edwards AFB, CA 93524, ashwani.vij@edwards.af.mil, (2) University of California, Riverside, (3) University of Southern California, Los Angeles, (4) Air Force Research Laboratory, Edwards and University of Southern California, Los Angeles, Edwards AFB, CA 93524, Fax: 661-275 5471, karl.christe@edwards.af.mil

The isomerization of trans- N_2F_2 to cis- N_2F_2 going through $N_2F^+AsF_6^-$ is unpredictable, erratic, requires 2 steps, and consumes an equimolar amount of AsF_5 . It was found that catalytic amounts of SbF_5 at 30C can achieve this isomerization, but still result in substantial N_2F_2 losses due to $N_2F^+SbF_6^-$ formation. When the reaction is carried out at 60C, surprisingly $NF_4^+SbF_6^-$. $nSbF_5$ is formed. The crystal structures of $N_2F^+SbF_6^-$ (disordered), $N_2F^+SbF_6^-$ (disordered), $N_2F^+SbF_6^-$ (ordered), and $NF_4^+Sb_2F_{11}^-$ were determined and are discussed. AlF_3 was also studied as a catalyst for the N_2F_2 isomerization and was found to be an ideal catalyst resulting in very high conversions of trans- N_2F_2 and high yields of cis- N_2F_2 . The AlF_3 can be used repeatedly without loss of activity or N_2F^+ salt formation. Cis- N_2F_2 forms with SnF_4 at low temperatures a 2:1 salt, $(N_2F^+)2SnF_6^{-2-}$, that slowly loses N_2F_2 at room temperature to give $N_2F^+SnF_5^-$. The crystal structure of $H_3NF^+CF_3SO_3^-$ was also determined and exhibits a relatively long N_2F^- bond.

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